Classification of phase transitions of finite Bose-Einstein condensates in power law traps by Fisher zeros

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We present a detailed description of a classification scheme for phase transitions in finite systems based on the distribution of Fisher zeros of the canonical partition function in the complex temperature plane. We apply this scheme to finite Bose-systems in power law traps within a semi-analytic approach with a continuous one-particle density of states $\Omega(E) \sim E^{d-1}$ for different values of d and to a three dimensional harmonically confined ideal Bose-gas with discrete energy levels. Our results indicate that the order of the Bose-Einstein condensation phase transition sensitively depends on the confining potential.

I. INTRODUCTION

In 1924 S. Bose and A. Einstein predicted that in a system of bosons at temperatures below a certain critical temperature T_C the single-particle ground state is macroscopically occupied [1]. This effect is commonly referred as Bose-Einstein condensation and a large number of phenomena, among others the condensation phenomena in alkali atoms, the superfluidity of ^{4}He and the superconductivity, are identified as signatures of this effect. However, the physical situation is very intricate in most experiments.

Recent experiments with dilute gases of alkali atoms in magnetic [2] and optical [3] traps are in some sense the up to now best experimental approximation of the ideal non-interacting Bose-Einstein system in an external power law potential. The achievement of ultra-low temperatures by laser cooling and evaporative cooling opens the opportunity to study the Bose-Einstein condensation under systematic variation of adjustable external parameters, e.g the trap geometry, the number of trapped atoms, the temperature, and by the choice of the alkali atoms the effective interparticle interactions. Even in the approximation of non-interacting particles the explanation of these experiments requires some care, because the number of bosons in these novel traps is finite and fixed and the standard grand-canonical treatment is not appropriate. The effect of the finite particle numbers on the second moments of the distribution function, e.g. the specific heat and the fluctuation of the ground state occupation number has been addressed in a number of publications [4, 5]. In [4, 6] we have presented a recursion method to calculate the canonical partition function for non-interacting bosons and investigated the dependency of the thermodynamic properties of the condensate on the trap geometry.

The order of the phase transition in small systems sensitively depends on finite size effects. Compared to the macroscopic system even for as simple systems as the 3-dimensional ideal gas the order of the phase transition might change for mesoscopic systems where the number of particles is finite or for trapped gases with different trap geometries.

In this paper we address the classification of the phase transition of a finite number of non-interacting bosons in a power law trap with an effective one-particle density of states $\Omega(E) = E^{d-1}$ being formally equivalent to a d-dimensional harmonic oscillator or a $2d$-dimensional ideal gas. We use a classification scheme based on the distribution of zeros of the canonical partition function initially developed by Grossman *et al.* [7], and Fisher *et al.* [8], which has been extended by us [9] as a classification scheme for finite systems. On the basis of this classification scheme we are able to extract a qualitative difference between the order of the phase transition occuring in Bose-Einstein condensates in 3-dimensional traps [10, 11] and in 2-dimensional traps which was recently discovered by Safonov *et al.* in a gas of hydrogen atoms absorbed on the surface of liquid helium [12]. Since we do not consider particle interactions this difference is only due to the difference in the confining potential.

We give a detailed review of the classification scheme in Sec. II. In Sec. III we present the method for the calculation of the canonical partition function in the complex plane and describe details of the numerical implementation. Our results for $d = 1 - 6$ and particle numbers varying from 10 to 300 are presented in Sec. III as well as calculations for a 3-dimensional parabolically confined Bose-gas.

II. CLASSIFICATION SCHEME

In 1952 Yang and Lee have shown that the grand canonical partition function can be written as a function of its zeros in the complex fugacity plane, which lie for systems with hard-core interactions and for the Ising model on a unit circle [13].

Grossmann *et al.* [7] and Fisher [8] have extended this approach to the canonical ensemble by analytic continuation of the inverse temperature to the complex plane $\beta \to \mathcal{B} = \beta + i\tau$. Within this treatment all phenomenologically known types of phase transitions in macroscopic systems can be identified from the properties of the distribution of zeros of the canonical partition function.

In [9] we have presented a classification scheme for fi-

nite systems which has its macroscopic equivalent in the scheme given by Grossmann. As usual the canonical partition function reads

$$Z(\mathcal{B}) = \int \mathrm{d}E \ \Omega(E) \ \exp(-\mathcal{B}E), \qquad (1)$$

which we write as a product $Z(\mathcal{B}) = Z_{\lim}(\mathcal{B})Z_{\mathrm{int}}(\mathcal{B})$, where $Z_{\lim}(\mathcal{B})$ describes the limiting behavior of $Z(\mathcal{B})$ for $T \to \infty$ imposing that $\lim_{T \to \infty} Z_{\mathrm{int}}(\mathcal{B}) = 1$. This limiting partition function will only depend on the external potential applied to the system, whereas $Z_{\mathrm{int}}(\mathcal{B})$ will depend on the specific interaction between the system particles. E.g. for a N-particle system in a d-dimensional harmonic trap $Z_{\lim}(\mathcal{B}) = \mathcal{B}^{-dN}$ and thus the zeros of $Z(\mathcal{B})$ are the same as the zeros of $Z_{\mathrm{int}}(\mathcal{B})$. Since the partition function is an integral function, the zeros $\mathcal{B}_k = \mathcal{B}_{-k}^* = \beta_k + i\tau_k$ ($k \in \mathbb{N}$) are complex conjugated and the partition function reads

$$\begin{aligned} Z(\mathcal{B}) \ = \ & Z_{\lim}(\mathcal{B}) \ Z_{\mathrm{int}}(0) \ \exp(\mathcal{B}\partial_\mathcal{B} \ln Z_{\mathrm{int}}(0)) \\ & \times \prod_{k \in \mathbb{N}} \left(1 - \frac{\mathcal{B}}{\mathcal{B}_k}\right)\left(1 - \frac{\mathcal{B}}{\mathcal{B}_k^*}\right) \exp\left(\frac{\mathcal{B}}{\mathcal{B}_k} + \frac{\mathcal{B}}{\mathcal{B}_k^*}\right) \end{aligned} (2)$$

The zeros of $Z(\mathcal{B})$ are the poles of the Helmholtz free energy $F(\mathcal{B}) = -\frac{1}{\mathcal{B}} \ln Z(\mathcal{B})$, i.e. the free energy is analytic everywhere in the complex temperature plane except at the zeros of $Z(\mathcal{B})$.

Different phases are represented by regions of holomorphy which are separated by zeros lying dense on lines in the complex temperature plane. In finite systems the zeros do not squeeze on lines which leads to a more blurred separation of different phases. We interpret the zeros as boundary posts between two phases. The distribution of zeros contains the complete thermodynamic information about the system and all thermodynamic properties are derivable from it. Within this picture the interaction part of the specific heat is given by

$$C_{V,\mathrm{int}}(\mathcal{B}) = -k_\mathrm{B}\mathcal{B}^2 \sum_{k \in \mathbb{N}} \left[\frac{1}{(\mathcal{B}_k - \mathcal{B})^2} + \frac{1}{(\mathcal{B}_k^* - \mathcal{B})^2}\right]. \quad (3)$$

The zeros of the partition function are poles of $C_V(\mathcal{B})$. As can be seen from Eq. (3) a zero approaching the real axis infinitely close causes a divergence at real temperature. The contribution of a zero $\mathcal{B}_k$ to the specific heat decreases with increasing imaginary part τ_k. Thus, the thermodynamic properties of a system are governed by the zeros of Z close to the real axis.

The basic idea of the classification scheme for phase transitions in small systems presented in [9] is that the distribution of zeros close to the real axis can approximately be described by three parameters, where two of them reflect the order of the phase transition and the third merely the size of the system.

We assume that the zeros lie on straight lines (see Fig. 1) with a discrete density of zeros given by

$$\phi(\tau_k) = \frac{1}{2}\left(\frac{1}{|\mathcal{B}_k - \mathcal{B}_{k-1}|} + \frac{1}{|\mathcal{B}_{k+1} - \mathcal{B}_k|}\right), \qquad (4)$$
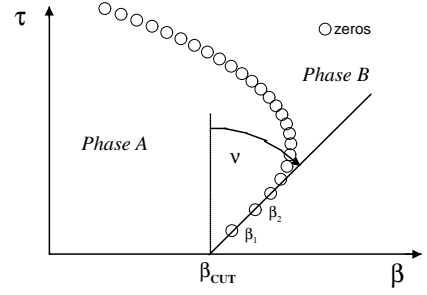

FIG. 1: Schematic illustration of the zeros in the complex temperature plane.

with $k = 2, 3, 4, \cdots$, and approximate for small τ the density of zeros by a simple power law $\phi(\tau) \sim \tau^\alpha$. Considering only the first three zeros the exponent α can be estimated as

$$\alpha = \frac{\ln \phi(\tau_3) - \ln \phi(\tau_2)}{\ln \tau_3 - \ln \tau_2}. \qquad (5)$$

The second parameter to describe the distribution of zeros is given by $\gamma = \tan \nu \sim (\beta_2 - \beta_1)/(\tau_2 - \tau_1)$ where ν is the crossing angle of the line of zeros with the real axis (see Fig. 1). The *discreteness* of the system is reflected in the imaginary part τ_1 of the zero closest to the real axis.

In the thermodynamic limit we have always $\tau_1 \to 0$. In this case the parameters α and γ coincide with those defined by Grossmann *et al* [7], who have shown how different types of phase transitions can be attributed to certain values of α and γ. They claimed that $\alpha = 0$ and $\gamma = 0$ corresponds to a first order phase transition, second order transitions correspond to $0 < \alpha < 1$ with $\gamma = 0$ or $\gamma \neq 0$, third order transitions to $1 \leq \alpha < 2$ with arbitrary values of γ, and that all higher order phase transition correspond to $\alpha > 1$. For macroscopic systems (with $\tau_1 \to 0$) α cannot be smaller than zero, because this would cause a divergence of the internal energy. However in small systems with a finite τ_1 this is possible.

In our classification scheme we therefore define phase transitions in small systems to be of first order for $\alpha \leq 0$, while second and higher order transitions are defined in complete analogy to the Grossmann scheme augmented by the third parameter τ_1. The definition of a critical temperature β_C in small systems is crucial and ambiguous since no thermodynamic properties diverge. Thus, different definitions are possible. We define the critical temperature as $\beta_{\mathrm{cut}} = \beta_1 - \gamma\tau_1$, i.e. the crossing point of the approximated line of zeros with the real temperature axis. An alternative definition is the real part of the first complex zero β_1. In the thermodynamic limit both definitions coincide.

Comparing the specific heats calculated for different discrete distributions of zeros shows the advantages of this classification scheme. Fig. 2 shows (a) three distributions of zeros lying on straight lines corresponding to a first order transition ($\alpha = 0$ and $\gamma = 0$), a second order

transition ($\alpha = 0.5$ and $\gamma = -0.5$), and a third order phase transition ($\alpha = 1.5$ and $\gamma = -1$) and (b) the pertinent specific heats. In all cases the specific heat exhibit a hump extending over a finite temperature region and cannot be used to classify the phase transition. In contrast, even for very small systems (large τ_1) the order of the phase transition is extractable from the distribution of zeros.
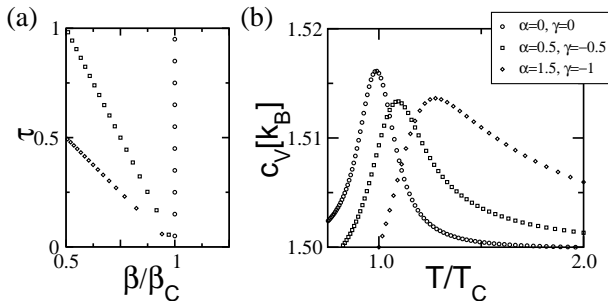

FIG. 2: Plot of (a) generated zeros lying on straight lines to simulate first ($\alpha = 0$ and $\gamma = 0$), second ($\alpha = 0.5$ and $\gamma = -0.5$), and third ($\alpha = 1.5$ and $\gamma = -1$) order phase transitions and (b) the appropriate specific heats per particle.

The zeros of the canonical partition function have a distinct geometrical interpretation which explains the smoothed curves of the specific heat and other thermodynamic properties in finite systems.

Fig. 3 shows (a) the ground state occupation number $|\eta_0(\mathcal{B})|/N$ in the complex temperature plane and (b) the ground state occupation number at real temperatures for a finite ideal Bose gas of $N = 120$ particles, where $\eta_0(\mathcal{B})$ is given by the derivative of the logarithm of the canonical partition function $Z(\mathcal{B})$ with respect to the ground state energy ϵ_0, i.e. $\eta_0(\mathcal{B}) = -\frac{1}{\mathcal{B}} \partial_{\epsilon_0} Z(\mathcal{B})/Z(\mathcal{B})$.
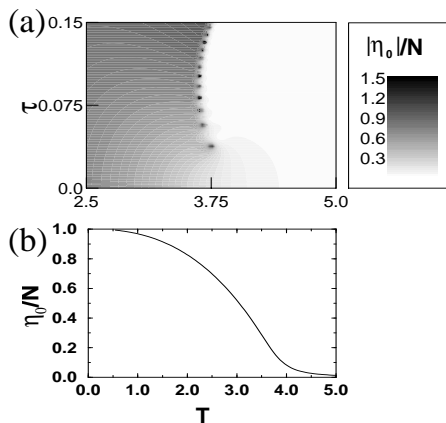

FIG. 3: Comparison of (a) $|\eta_0|/N$ with (b) the appropriate value of η_0 at real temperatures for a 120 particle harmonically trapped ideal Bose-gas (note that $\hbar = k_B = \omega = 1$).

Zeros of the partition function are poles of $\eta_0(\mathcal{B})$ and are indicated by dark spots, which influence the value

of the ground state occupation number at real temperatures impressively. Every pole seems to *radiate* onto the real axis and therefore determines the occupation number at real temperatures. This *radiation* extends over a broad temperature range so that the occupation number for real temperatures does not show a discontinuity but a smoothed curve. A closer look at Eq. (3) gives the mathematical explanation for this effect. The discrete distribution of zeros, i.e. $\tau_1 > 0$, inhibits the specific heat and all other thermodynamic properties to show a divergency at some critical temperature because the denominators of the arguments of the sum remain finite.

Without going into a detailed analysis we note that in the thermodynamic limit the parameter α is connected to the critical index for the specific heat by

$$C_V \sim (\beta - \beta_c)^{\alpha-1}. \tag{6}$$

However, since critical indices are used to describe the shape of a divergency at the critical point an extension to small systems seems to be more or less academical.

The introduction of complex temperatures might seem artificial at first sight but, in fact, the imaginary parts τ_k of the complex zeros $\mathcal{B}_k$ have an obvious quantum mechanical interpretation. We write the quantum mechanical partition function as

$$
\begin{aligned}
Z(\beta + i\tau/\hbar) &= \mathrm{Tr}(\exp(-i\tau\hat{H}/\hbar)\exp(-\beta\hat{H})) \quad (7)\\
&= \left\langle \Psi_{\mathrm{can}} | \exp(-i\tau\hat{H}/\hbar) | \Psi_{\mathrm{can}} \right\rangle \quad (8)\\
&= \left\langle \Psi_{\mathrm{can}}(t=0) | \Psi_{\mathrm{can}}(t=\tau) \right\rangle, \quad (9)
\end{aligned}
$$

introducing a *canonical state* as a sum over Boltzmann-weighted eigenstates $|\Psi_{\mathrm{can}}\rangle = \sum_k \exp(-\beta\epsilon_k/2)|\phi_k\rangle$. We explicitly write the imaginary part as $\tau/\hbar$ since the dimension is $1/[\text{energy}]$ and the imaginary part therefore can be interpreted as time. Then the imaginary parts τ_k of the zeros resemble those times for which the overlap of the initial canonical state with the time evolved state vanishes. However, they are not connected to a single system but to a whole ensemble of identical systems in a heat bath with an initial Boltzmann distribution.

III. BEC IN POWER LAW TRAPS

In this section we assume a continuous single particle density of states $\Omega(E) = E^{d-1}$ as an approximation for a d-dimensional harmonic oscillator or a $2d$-dimensional ideal gas. E.g. for the harmonic oscillator this corresponds to the limit of $\hbar\omega \to 0$ and taking only the leading term of the degeneracy of the single particle energy levels. The one-particle partition function is given by the Laplace transformation

$$Z_1(\mathcal{B}) = \int dE \, E^{d-1} \exp(-\mathcal{B}E) = (d-1)! \, \mathcal{B}^{-d}. \tag{10}$$

The canonical partition function for N non-interacting bosons can be calculated by the following recursion [6]

$$Z_N(\mathcal{B}) = \frac{1}{N} \sum_{k=1}^{N} Z_1(k\mathcal{B}) \, Z_{N-k}(\mathcal{B}), \qquad (11)$$

where $Z_1(k\mathcal{B}) = \sum_i \exp(-k\mathcal{B}\epsilon_i)$ is the one-particle partition function at temperature $k\mathcal{B}$ and $Z_0(\mathcal{B}) = 1$. For small particle numbers this recursion works fine, even though its numerical effort grows proportional to N^2.

With (10) as Z_1 Eq. (11) leads to a polynomial of order N in $(1/\mathcal{B})^d$ for Z_N which can be easily generated using MAPLE or MATHEMATICA. The zeros of this polynomial can be found by standard numerical methods.
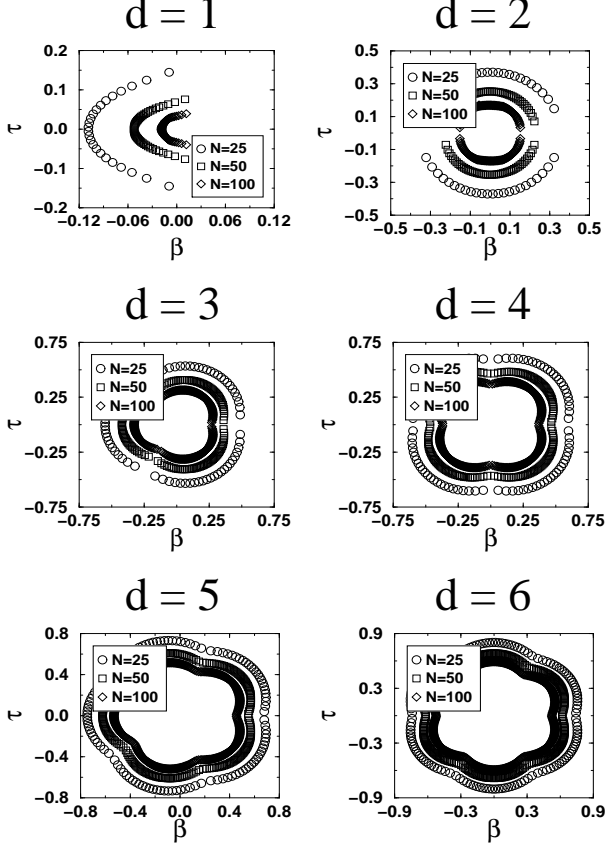

FIG. 4: Distribution of zeros for Bose-Einstein Condensates with continuous one-particle density of states $\Omega(E) = E^{d-1}$ for $d = 1 - 6$.

Fig. 4 displays the zeros of the N-particle partition function for $d = 1 - 6$ in the complex temperature plane for particle numbers $N = 25, 50$ and 100. For $d = 2 - 6$ the zeros approach the positive real axis with increasing particle number and are shifted to higher temperatures which is already at first sight an indicator of phase transitions. For $d = 1$ the zeros approach the real axis only at negative temperature. This behavior is consistent with the usual prediction that there is no Bose-Einstein condensation for the one-dimensional harmonic oscillator and the two-dimensional ideal Bose gas [10].
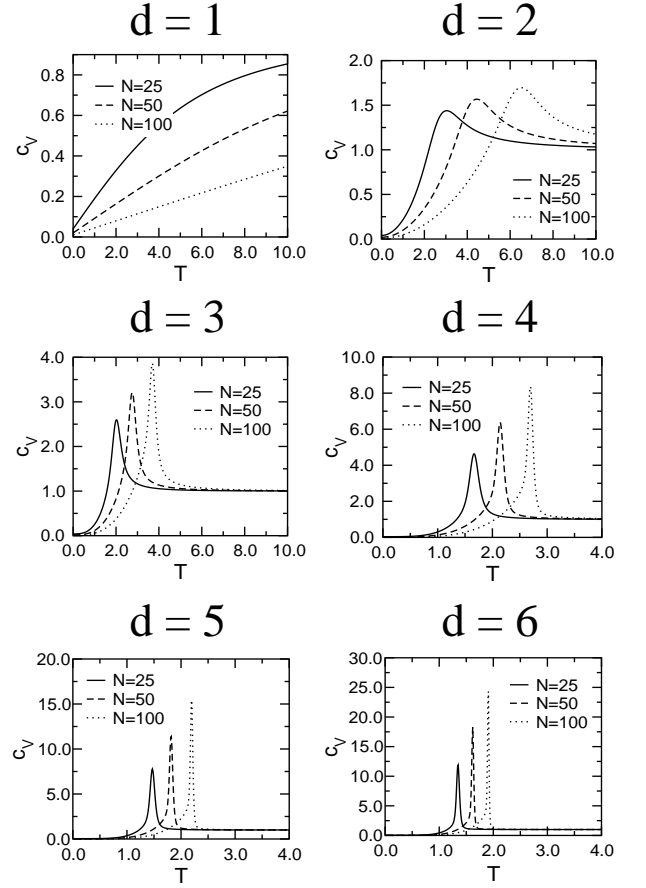

FIG. 5: Specific heat scaled by dN of Bose-Einstein Condensates with continuous one-particle density of states for $d = 1 - 6$.

The symmetry of the distributions of zeros is due to the fact that Z_N is a polynomial in $\mathcal{B}^{-d}$. For this reason it can be inferred that for $d \to \infty$ the zeros lie on a perfect circle.

Fig. 5 shows the corresponding specific heats calculated using equation (3). As expected, for $d = 1$ the specific heat has no hump and approaches with increasing temperature the classical value. We therefore expel the analysis of $d = 1$ from the discussions below. For $d = 2-6$ the specific heats show humps or peaks, which get sharper with increasing d and increasing particle number. However, from these smooth curves the orders of the phase transition cannot be deduced.

In Fig. 6 the classification parameters α, γ, τ_1 defined above are plotted for two to six dimensions and particle numbers up to $N = 100$. For all values of d the parameter α is only a slightly varying function of N and approaches very fast an almost constant value. Since α is the primary classification parameter from Fig. 6(a) we can directly infer that the $d = 2$ system exhibits a third order phase transition ($\alpha > 1$) while the transition for all higher dimensions is of second order ($0 \leq \alpha \leq 1$). For $N = 50$ the dependence of α on d is plotted in Fig. 7(a). Since α decreases rather rapidly with increas-
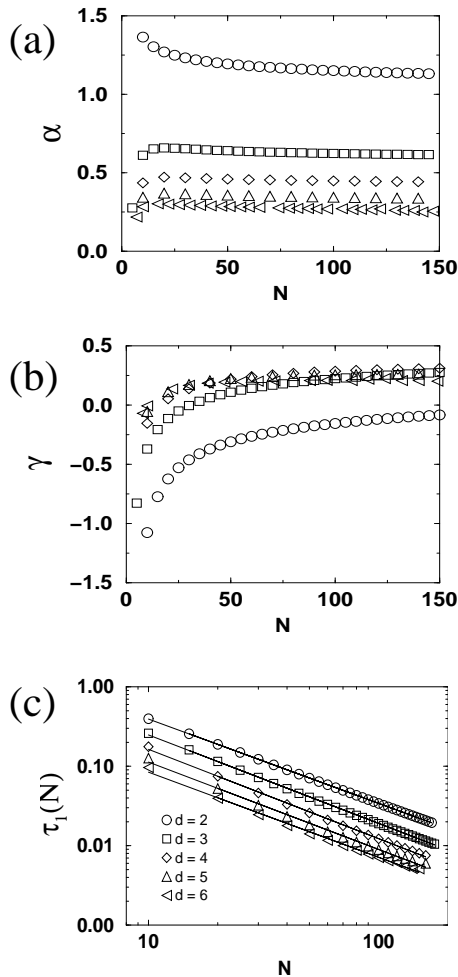
FIG. 6: Classification parameters α, γ and τ_1 for $d = 2 - 6$ versus particle numbers N.

ing d it can be speculated that systems corresponding to a large d exhibit a phase transition which is almost of first order. As mentioned above for finite systems even values $\alpha \leq 0$ cannot be excluded by mathematical reasons. We note that two-dimensional Bose-gases are an interesting and growing field of research. As it is well known, the ideal free Bose-gas in two dimensions ($d = 1$) does not show a phase transition due to thermal fluctuations which destabilize the condensate [14]. Switching on a confining potential greatly influences the properties of the gas, the thermal fluctuations are suppressed and the gas will show Bose-Einstein condensation. Recent experiments [12] have shown that Bose-Einstein condensation is possible even though it is called a quasi-condensate. In our notion the quasi-condensate is just a third order phase transition. Thus, our results are in complete agreement with recent experiments and earlier theoretical work. An interesting question in this respect is whether the order of the transition changes for $d = 2$ in the limit $N \to \infty$. Additional calculation for larger N, which are not printed in Fig. 6 indicate that

α approaches 1 or might even get smaller. Note that $d = 2$ is equivalent to a hypothetical 4-dimensional ideal Bose gas or Bosons confined in a 2-dimensional parabolic trap. Our results indicate that the order of the phase transition sensitively depends on d for values around 2. This might be the reason why phase transitions in three space dimensions are sometimes classified as second and sometimes as third order phase transitions.

The parameter τ_1 is a measure of the finite size of the system, i.e. the scaling behavior of τ_1 as a function of N is a measure of how fast a system approaches a true n-th order phase transition in the Ehrenfest sense. The N dependence of τ_1 is displayed in Fig. 6(c). The scaling behavior can be approximated by $\tau_1 \sim N^{-\delta}$ with δ ranging between 1.06 and 1.12 for $d = 2 - 6$.

The d dependence of the classification parameter is visualized in Fig. 7 for 50 particles. For this system size we found $\alpha \sim d^{-4/3}$ and $\tau_1 \sim d^{-4/3}$.
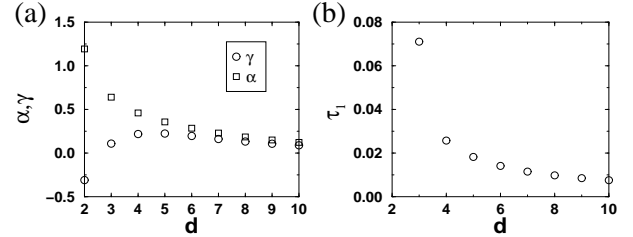

FIG. 7: Classification parameters for $N = 50$ for different densities of states $\Omega(E) = E^{d-1}$ and $d = 2 - 10$.
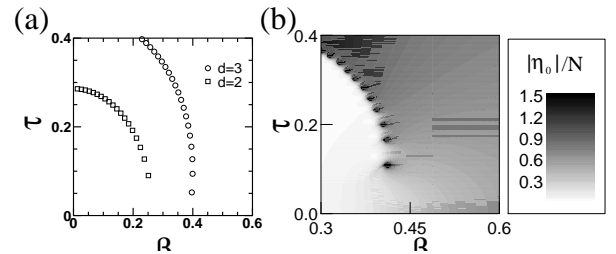

FIG. 8: Comparison between calculated zeros of the canonical partition function for three dimensional trap geometries with (a) a continuous single-particle densities of states and (b) discrete energy levels for $N = 40$.

The results presented above for continuous single particle densities of states $\Omega(E) = E^{d-1}$ are obtained within semi-analytical calculations. In order to compare these results to systems with a discrete level density we adopt as a reference system the 3-dimensional harmonic oscillator with the partition function given by

$$Z(\mathcal{B}) = \sum_{n=0}^{\infty} \frac{(n+2)(n+1)}{2} \exp(-\mathcal{B}(n+3/2)), \quad (12)$$

with $\hbar = \omega = k_B = 1$.

Fig. 8(a) displays the zeros of the partition function (10) for $d = 2$ and $d = 3$. Fig. 8(b) displays a contour

plot of the absolute value of the ground state occupation number $\eta_0(\mathcal{B}) = -\frac{1}{\mathcal{B}}\partial_{\epsilon_0} Z(\mathcal{B})/Z(\mathcal{B})$ with Z given by (12) calculated using an alternative recursion formula [4]. The zeros of Z are poles of η_0 and are indicated by dark spots in this figure.

Analyzing the distribution of zeros consolidates our speculation that the order of the phase transition sensitively depends on d. The distribution of zeros behaves like the above calculated values for $d = 2$ but quantitatively like $d = 3$. Since the degeneracy of the three-dimensional harmonically confined ideal Bose-gas is a second-order polynomial not only the quadratic term has to be taken into account. The linear term becomes dominant for lower temperatures, so for very low temperatures the best approximation of a continuous one-particle density of states is $\Omega(E) = E$. The parameter α supports this statement [9], i.e. α resides in a region above 1. Whereas the parameter γ behaves like the $d = 3$ case. Finally the parameter τ_1 which is a measure for the discreteness of the system shows a $\tau_1 \sim N^{-0.96}$ dependence which is comparable to the one for $d = 2$. Thus, for small systems the phase transition is of third order, it can be speculated if it becomes a second order transition in the thermodynamic limit.
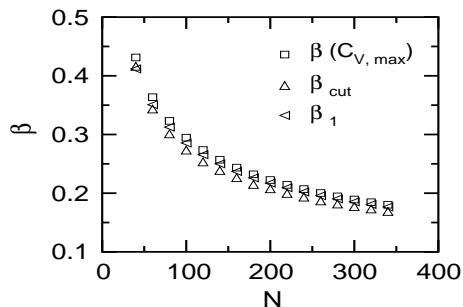

FIG. 9: Comparison between three different approaches to define a critical temperature for phase transitions in finite systems.

Not only qualitatively but also quantitatively our calculations are in very good agreement with recent theoretical works [15, 16]. Comparing the *critical* temperature which we defined in Sec. II with the usually utilized ones like the temperature of the peak of the specific heat $\beta(C_{V,max})$ or the grand-canonically calculated $T_C \sim N^{1/3}$ confirms our approach. In Fig. 9 three possible definitions of the critical temperature are given which all coincide in the thermodynamic limit. All definitions show a $\beta \sim N^{-\rho}$ dependence with ρ ranging between 2/5 and 1/3.

IV. CONCLUSION

Starting with the old ideas of Yang and Lee, and Grossmann *et al.* we have developed a classification scheme for phase transitions in finite systems. Based on the analytic continuation of the inverse temperature β into the complex plane we have shown the advantages of this approach. The distribution of the so-called Fisher-zeros $\mathcal{B}_k$ draws enlightening pictures even for small systems whereas the usually referred thermodynamic properties like the specific heat fail to classify the phase transitions properly. The classification scheme presented in this paper enables us to name the order of the transition in a non-ambiguous way. The complex parts τ_k of the zeros $\mathcal{B}_k$ resemble times for which a whole ensemble of identical systems under consideration in a heat bath with an initial Boltzmann-distribution looses its memory.

We have applied this to ideal non-interacting Bose-gases confined in power-law traps. We have found that the order of the phase transition sensitively depends on the single particle density of states generated by the confining potential. The distribution of zeros exactly reveals the order of the phase transition in finite systems.

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